Ionization potential depression in hot dense plasmas through a pure classical model

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November 7, 2014

Abstract

The ionization potential of an ion embedded in a plasma is lowered due to the whole charged particles (ions and electrons) interacting with that ion. It is the so called plasma effect. The numerical plasma model developed years ago, based on classical molecular dynamics, capable to describe a neutral plasma at equilibrium involving ions of various charge states of the same atom together with electrons, is used to investigate the ionization potential depression (IPD). The study of the IPD is illustrated and discussed for aluminum plasmas at mid and solid density and electron temperatures varying from 50eV to 190eV. The method relies on a sampling of the total potential energy of the electron located at an ion being ionized. The potential energy of such electron results from the whole interacting charged particles interacting with it.

1 Introduction

The radiative properties of an atom or an ion surrounded by a plasma are modified through various mechanisms. For instance the line shapes of radiations emitted by bound-bound transitions are broadened and therefore carry informations useful for plasma diagnostics. Depending on plasma conditions the electrons supposedly occupying the upper quantum levels of radiators no longer exist as they belong to the plasma free electron population. All the charges present in the radiator environment, electrons and ions, contribute to the lowering of the energy required to free an electron in the fundamental state. This mechanism is known as ionization potential depression (IPD). The knowledge of IPD is useful as it affects both the radiative properties of the various ionic states and their populations. Its evaluation deals with highly complex n-body coupled systems, involving particles with different dynamics and attractive ion-electron forces. A few recent experiments [1, 2] leading to IPD measurements in situ renew interest for this issue. On the other hand some approximate models allow to discuss experiments

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as they provide a scaling for the IPD. This interest has motivated the development of an alternative approach. The present work on IPD is carried out using a classical molecular dynamics (MD) code, the BINGO-TCP code [3], developed recently to simulate neutral multi-component (various charge state ions and electrons) plasma. Our simulations involve a mechanism of collisional ionization/recombination necessary to simulate stationary plasmas with a definite temperature and equilibrated populations of ions of various charge states. The code, particularly robust and versatile, has to be understood as an efficient tool able to provide, although approximate, reference data available by sampling, once a stationary state of the plasma has been reached. All the advantages of classical MD techniques benefit to the present approach which relies on a reduced set of postulates regarding mainly an ion-electron potential depending on the ion charge state and an ionization-recombination protocol which controls the plasma ion charge distribution in the plasma and the trapping of electrons in the ion wells. The study focuses on aluminum plasmas for two ionic densities and several temperatures in order to explore the IPD for different plasma coupling conditions.

2 Model summaries

2.1 Theoretical models

The IPD has been formulated in the sixties following two slightly distinct ways. First Stewart and Pyatt [4] propose a model formulated using the finite-temperature Thomas-Fermi potential for the average electrostatic potential near nuclei of the plasma particles. The bound electrons are considered as part of the unperturbed ion, the plasma free electrons are described by Fermi-Dirac statistics and ions by Maxwell-Boltzmann statistics. Note that in this model, the bound electrons do not contribute to the reduction of the ionization energy. The reduction of the ionization energy is given by:

$$\Delta U_{SP}(Z) = \frac{3Ze^2}{2r_0}\left\{ \left[1 + (\frac{\lambda_D}{r_0})^3\right]^{2/3} - (\frac{\lambda_D}{r_0})^2 \right\} \tag{1}$$

$$\lambda_D = \sqrt{\frac{kT}{4\pi(n_i + n_e)e^2}},\ \frac{4\pi n_i r_0^3}{3} = 1 \tag{2}$$

where Z is the charge state of the atom (or ion) after the ionization occurrence, i.e. $Z = 1$ for neutrals, λ_D is a generalized Debye length and r_0 the average inter-ionic distance for the average ion charge $\overline{Z}$. n_i is the corresponding ion density and n_e the electron density. In the high density or low temperature limit, the IPD becomes:

$$\Delta U_{SP}(Z) = \frac{3Ze^2}{2r_0} \tag{3}$$

Second, Ecker-Kröll [5] formulated a generalized Saha equation as a function of the chemical potential of the plasma. This model assumes two functional forms for the IPD depending on the particle (ions plus electrons) density:

$$\Delta U_{EK}(Z) = Ze^2 \begin{cases} 1/\lambda_D & n_{cr} \geq n_i(1+\overline{Z}) \\ C \times (1+\overline{Z})^{1/3}/r_0 & n_{cr} < n_i(1+\overline{Z}) \end{cases} \tag{4}$$

where

$$n_{cr} = \frac{3}{4\pi}\left(\frac{kT}{Z_N^2 e^2}\right)^3 \tag{5}$$

is the critical density which includes both ion and free electron densities, Z_N being the nuclear charge and T the plasma temperature. The constant C is determined by imposing the continuity of the IPD at the critical density:

$$C = \left(\frac{r_0}{(1+\overline{Z})^{1/3}\lambda_D}\right)_{n_{cr}}. \tag{6}$$

Recent experimental results [1] have shown discrepancies with the SP model which is the most widely used among the IPD models and, shown good agreement with the EK model in which C has been set to 1 according to experimental considerations. In contrast, other experimental results [2] obtained independently have corroborated the SP model. In the following, we will compare our simulation results with both models SP and EK with $C = 1$.

2.2 Molecular dynamics, potentials and ionization/recombination protocol

The BINGO-TCP code is based on standard MD techniques. The particle motions in the simulation box is ruled by a Verlet velocity algorithm associated with periodic boundary conditions. The whole interactions between charges contribute to the motion of electrons and ions. The time step is necessarily chosen for an accurate description of electron motion. The total charge in the box is zero. The Born-Oppenheimer approximation is useless and collectives behaviors naturally appear. The BINGO-TCP code involves two major features intended to achieve simulations of plasmas close to real, with ion charge distributions adjusting with temperature and density conditions.

First, a regularized electron/ion potential, i.e., finite at short distances, depending on the ion charge Z_i is set up as:

$$V_{ie}(r) = -Z_i e^2 e^{-r/\lambda}(1 - e^{-r/\delta(Z_i)})/r \tag{7}$$

where the regularization distance $\delta(Z_i)$ is function of the ionization energy E_i of an ion of charge Z_i. In other words an electron located at an ion ($r = 0$) occupies the fundamental state of the ion whose charge is Z_i with a core charge $Z_i + 1$.

$$\delta(Z_i) = Z_i e^2/E_i \tag{8}$$

Ion-ion and electron-electron potentials are taken to be Coulomb potentials

$$V_{ii,ee} = Z_{i,e}^2 e^2 e^{-r/\lambda}/r \tag{9}$$

The screening factor present in these potentials $e^{-r/\lambda}$ where λ is half the simulation box size, helps to smooth the small fluctuations of forces arising with the periodic boundary conditions. It doesn't affect the mechanisms controlling the particle motion in the simulation box.

Second, the collisional ionization/recombination process implemented in the code has two fundamental functions. In the one hand, it allows the evolution of the charge state population towards a stationary state depending on temperature, density and composition of the plasma. In the second hand, it favors the setting up of a population of electrons temporary trapped in the ion wells. Briefly, the local conditions for the ionization of an ion of charge Z_i are controlled by the total energy E and the location, inside a shell around the ion, of the two nearest neighbor electrons of that ion. If $E > 0$, Z_i is replaced by $Z_i + 1$ and an electron appears at the same location as the ion being ionized. This electron-ion pair stands for the fundamental state of Z_i. The effective ionization, i.e., the heating of the supplementary electron is a long term process resulting from the multiple interactions in the simulation box. An analog process occurs for the collisional recombination of an electron when $E < 0$. The sign of the total energy of individual electrons provides a simple way to separate the electron population into trapped (negative energy) and free (positive energy) electrons. Electron temperature and density are obtained on the basis of the free electron population.

The present work exploits the instantaneous setting of one supplementary electron at an ion starting an ionization process. The ionization protocol guarantees that there is no other electron at short distance from the ion undergoing an ionization. The magnitude of the supplementary electron potential energy represents the opposite amount of kinetic energy required by the electron to join the free electron population. Such events are rather seldom but sufficient to perform a statistical study of these energies for each kind of ion. Their average for each ionic charge state is interpreted as the corresponding IPD.

3 Results

The study of the IPD is illustrated and discussed for aluminum plasmas at two different densities ($\rho = 0.34$ g/cm^3 and $\rho = 2.7$ g/cm^3) and plasma temperatures varying from 50 eV to 190 eV. TCP-MD simulations have been performed with 80 atoms of aluminum. We started the simulations with an electronic density corresponding to a mean charge $\overline{Z} = 8$. After an equilibration step controlled by imposing the temperature, we ensure that an equilibrium state has been reached by checking the stationarity of the total energy and charge distributions.

The analysis of the electron energy distribution function permits to infer the electronic density and consequently the mean charge value $\overline{Z}$. Considering that the distribution function of negative energies is associated with trapped electrons and knowing the total number of electrons in the simulation box, this function allows us to estimate the density of free electrons in our simulations. The variation of the mean charge value as a function of the temperature has been plotted in fig. 1 and compared with the FLYCHK code [6] results. It can be observed that, except at the highest temperature, the mean charge value obtained by TCP-MD simulation is smaller than the one obtained by FLYCHK. Nevertheless, the agreement is good with an overall difference of less than 6.5 $\%$. At the solid density, it has been found that the mean ionization of the simulated plasmas was larger than that inferred by FLYCHK and that the overall difference was about 20 $\%$.

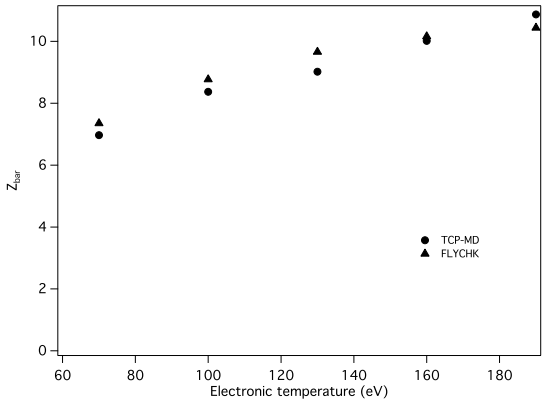

Figure 1: Mean charge value versus temperature at $\rho = 0.34$ g/cm^3.

By sampling the total potential energies of the electrons located at ions being ionized while they are in the same ionization stage (cf. fig. 2(a)), we have access to their corresponding average ionization energy. The difference with the ionization energy of the isolated ions can be interpreted as the corresponding IPD. The IPD of the different ion stages present in the simulated plasma has been measured for all the five cases of temperature at $\rho = 0.34$ g/cm^3, the results are plotted in fig. 2(b). It can be noticed that the statistics on the ionization events did not permit to measure the IPD for Z lower than 8. The IPD decreases as the temperature increases. The SP model presents a similar behavior but not the modified EK one which depends on the temperature only through the value of $\overline{Z}$.

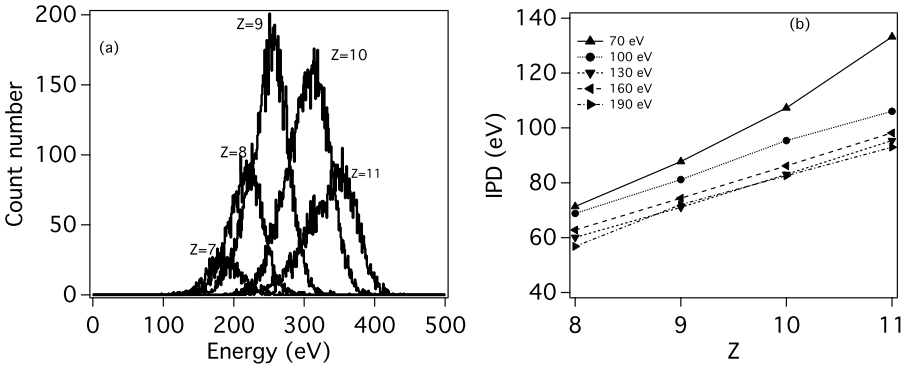

Figure 2: (a) Distribution of the total potential energy of an electron located at different charge state ions at 100 eV and $\rho = 0.34$ g/cm^3. (b) Evolution of the IPD with the temperature at $\rho = 0.34$ g/cm^3.

Figure 3 and 4 show the comparisons of the TCP-MD results with the SP and EK models at $\rho = 0.34$ g/cm^3 and $T_i = T_e = 100$ eV, and $\rho = 2.7$ g/cm^3 and $T_i = T_e = 50$ eV, respectively. As expected, the IPD is greater for the highest density and lowest temperature and it corresponds to a ionization energy 40% lower than the corresponding energy of the isolated ions. With $C = 1$ and the chosen conditions, the modified EK model gives IPD values greater than the SP predictions. For both cases, the simulated IPDs fall in between the two models. It can be seen in fig. 4 that the IPD compares well with the SP strong coupling limit. This limit does not depend on temperature, our calculation being performed at $T_i = T_e = 50$ eV, this result should be considered cautiously.

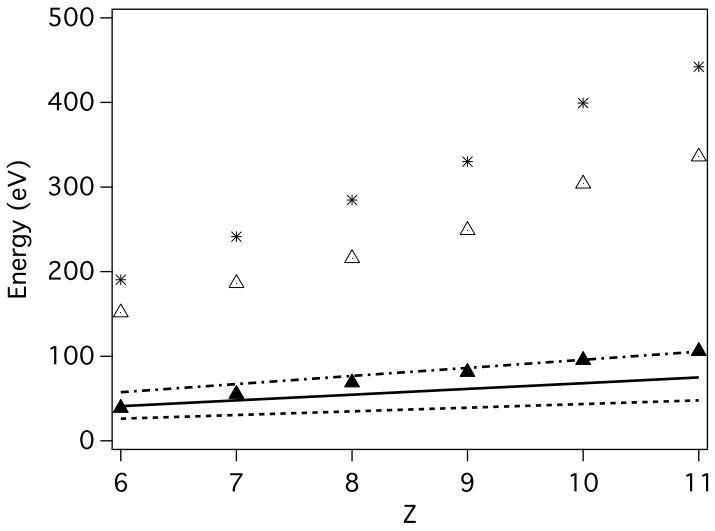

Figure 3: Comparison of the simulation results at 100 eV and $\rho = 0.34$ g/cm^3 with the SP and EK models. (stars): ionization energy of the isolated ion, (triangles): simulated ionization energy, (black triangles): simulated ionization potential depression, (dash-dotted line): modified EK model, (full line): SP strong coupling limit, (dashed line): SP model.

4 Conclusion

The ionization potential depression in a dense aluminum plasma has been simulated via a pure classical model based on classical molecular dynamics simulation method adapted to follow the evolution of plasmas involving ions of various charge states. Due to the specific implementation of the ionization/recombination model, our classical MD method gives access to the ionization potential of an ion accounting for the influence of the free electrons and neighboring ions. By comparison with the ionization potential

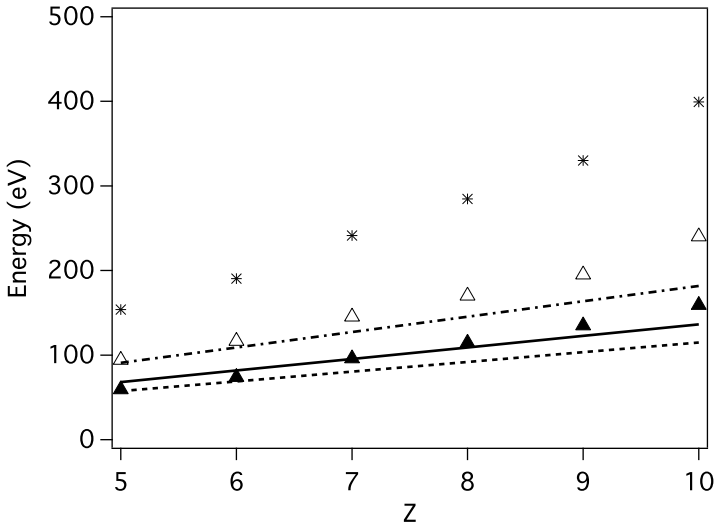

Figure 4: Comparison of the simulation results at 50 eV and $\rho = 2.7$ g/cm^3 with the SP and EK models. Same code as fig. 3.

of the equivalent isolated ions, the ionization potential depression can be estimated. Calculations have been performed at two ionic densities, $\rho = 0.34$ g/cm^3 and $\rho = 2.7$ g/cm^3 and for temperatures varying from 50 to 190 eV. First, It has been shown that the IPD depends on the temperature. Second, the results obtained with our TCP-MD simulation code have been compared with different semiclassical models, the SP model and the associated strong coupling limit which are widely used in astrophysical and laser plasma simulations, and the EK model which has been modified accordingly with Ciricosta's experimental results. It has been shown that the simulated IPD falls in between the SP and EK model results and compares well with the SP strong coupling limit for the highest density and lowest temperature. These first results are very encouraging. Owing to the fact that a bad estimation of the IPD in laser plasma simulations have consequences for the estimation of the ionization degree, the equation of state etc., the model proposed in this work appears as an important tool to provide data for further discussion on IPD models. In this context, the present results being obtained for stationary plasmas at equilibrium, the next step will be to simulate plasmas, with cold ions in order to compare with Ciricosta's experimental results.

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